Data Mining Exam

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Clustering
Introduction

Clustering is a way to categorize data to impose structure.

A use case is recommender systems (Amazon, Spotify, Netflix), where a user is recommended items that bought/listened to/watched by other users with similar interests.

Clustering
K-Means Optimization Problem

Given $D = (x_1, \ldots, x_n)$ where $x_i \in \mathbb{R}^p$, $K \in \mathbb{N}$ and let $C_1, \ldots, C_K$ denote different groups of the x_i's.

The K-Means algorithm tries to solve

$$\min_{C_1,\ldots,C_K} \left\{ \sum_{k=1}^{K} W(C_k) \right\}, \tag{1}$$

where $W(C_k)$ denotes the **within cluster variation**, in other words the dissimilarity of the group.

The most common dissimilarity measure is the is the squared Euclidean distance

$$W(C_k) := \frac{1}{|C_k|} \sum_{i,i' \in C_k} \sum_{j=1}^{p} (x_{i,j} - x_{i',j})^2. \tag{2}$$

Clustering
K-Means Optimization Problem

If we by $\bar{x}_{k,j} = \frac{1}{|C_k|} \sum_{i \in C_k} x_{i,j}$ denote the mean value of the j'th dimension in cluster k, it can be shown that

$$\frac{1}{|C_k|} \sum_{i,i' \in C_k} \sum_{j=1}^{p} (x_{i,j} - x_{i',j})^2 = 2 \sum_{i \in C_k} \sum_{j=1}^{p} (x_{i,j} - \bar{x}_{k,j})^2. \tag{3}$$

If we further note that $\bar{x}_{k,j} = \min_{\mu_k} \left\{ \sum_{i \in C_k} \sum_{j=1}^{p} (x_{i,j} - \mu_k)^2 \right\}$ this implies that the optimization problem in (1) can be rewritten as

$$\min_{C_1,\ldots,C_k,\mu_1,\ldots,\mu_k} \left\{ \sum_{k=1}^{K} \sum_{i \in C_k} \sum_{j=1}^{p} (x_{i,j} - \mu_k)^2 \right\}. \tag{4}$$

Clustering
K-Means Algorithm

The K-Means algorithm is now able to exploit the new formulation of the optimization problem and iteratively solve for $\{C_1, \ldots, C_k\}$ and $\{\mu_1, \ldots, \mu_k\}$.

This makes K-Means a greedy algorithm because, in each iteration it chooses optimal values for $\{C_1, \ldots, C_k\}$ and $\{\mu_1, \ldots, \mu_k\}$.

Convergence of the algorithm is therefore ensured, however we cannot guarantee it will find the global optimum.

Clustering
K-Means Algorithm

Algorithm 1: K-Means

```
1  Assign each obsevation to a cluster randomly
2  foreach Cluster do
3      Compute the centroid
4  foreach Observation do
5      Compute distance to all centroids
6      Assign to the closest
7  while Centroids have not changed since last iteration do
8      foreach Observation do
9          Compute distance to all centroids
10         Assign to the closest
11     foreach Cluster do
12         Compute the centroid
13 return Clusters
```

Clustering
An example of the K-Means algorithm

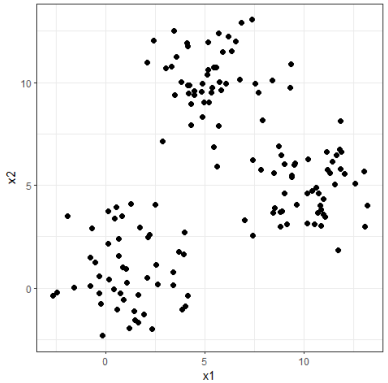


Figure: Iteration 01

Clustering
An example of the K-Means algorithm

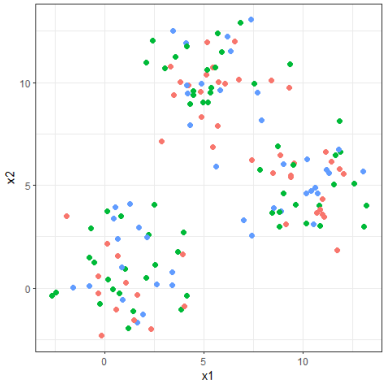


Figure: Iteration 02

Clustering
An example of the K-Means algorithm

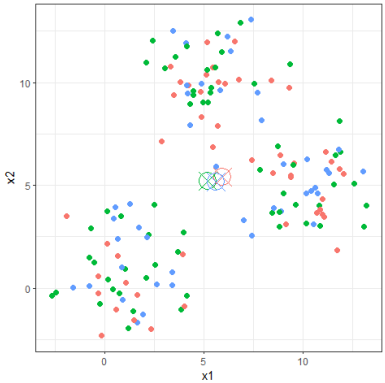


Figure: Iteration 03

Clustering

An example of the K-Means algorithm

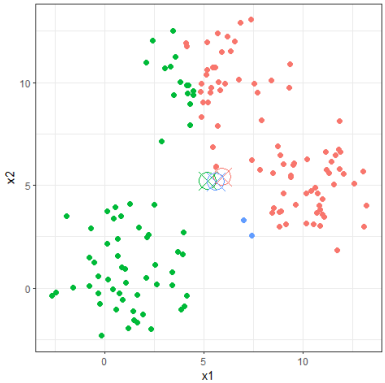


Figure: Iteration 04

Clustering
An example of the K-Means algorithm

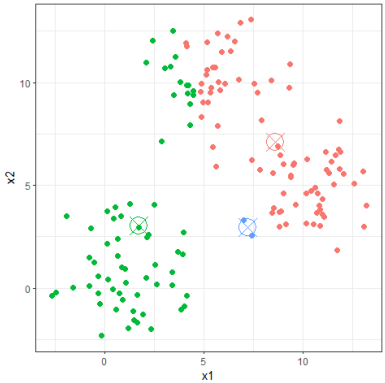


Figure: Iteration 05

Clustering
An example of the K-Means algorithm

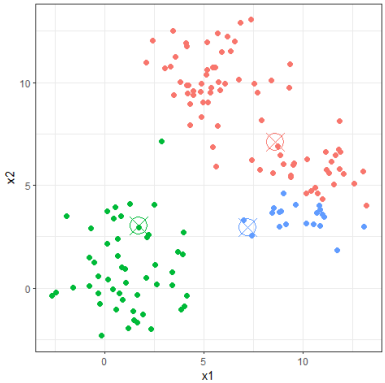


Figure: Iteration 06

Clustering
An example of the K-Means algorithm

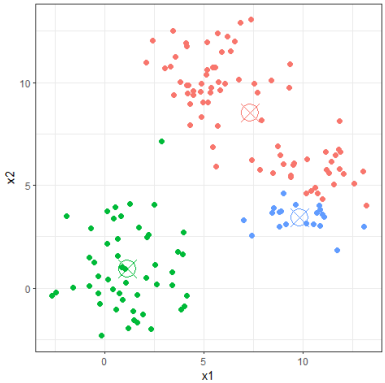


Figure: Iteration 07

Clustering
An example of the K-Means algorithm

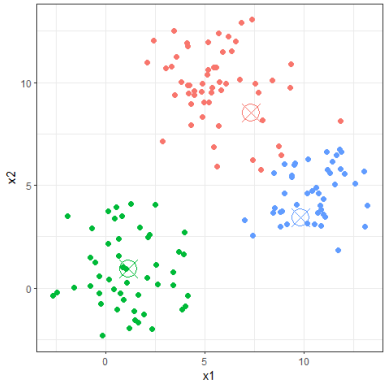


Figure: Iteration 08

Clustering
An example of the K-Means algorithm

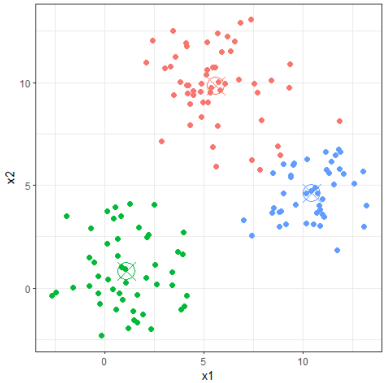


Figure: Iteration 09

Clustering
An example of the K-Means algorithm

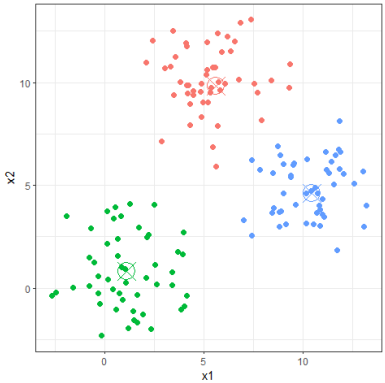


Figure: Iteration 10

Clustering
An example of the K-Means algorithm

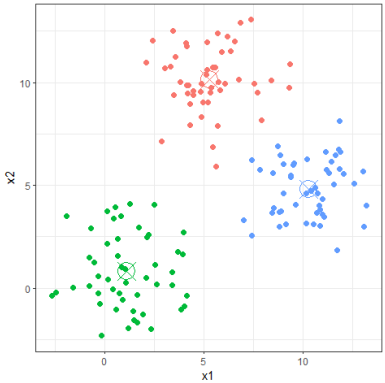


Figure: Iteration 11

Clustering
An example of the K-Means algorithm

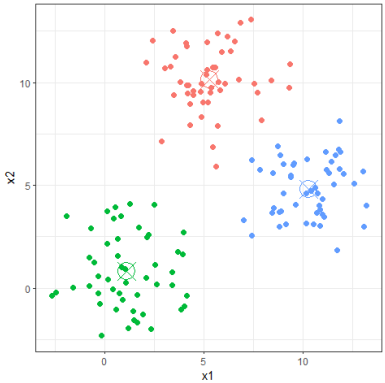


Figure: Iteration 12

Clustering
An example of the K-Means algorithm

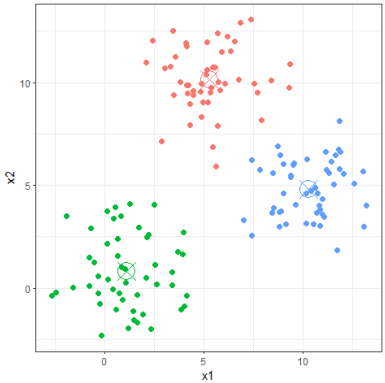


Figure: Iteration 13

Clustering
Number of clusters

Prior to running K-Means we need to determine the number of clusters. For some use cases this number may be predetermined by external factors. If the number of clusters is not predetermined, the data itself can indicate the optimal number.

The **total sum of squares** (total variance in the data) and the **within cluster sum of squares** are given by

$$SS_{total} = \sum_{i=1}^{n}(x_i - \bar{x})^2, \quad \bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i, \quad SS_{W_k} = \sum_{i \in C_k}(x_i - \bar{x}_k)^2, \quad \bar{x}_k = \frac{1}{n_k}\sum_{i \in C_k} x_i.$$

Then the **total within sum of squares** becomes $SS_W = \sum_{k=1}^{K} SS_{W_k}$. Using this we can calculate the **percentage of variance explained** as $PVE = 1 - SS_W / SS_{total}$.

Clustering
Number of clusters

We can then use what is called the **elbow method** to determine number of clusters.

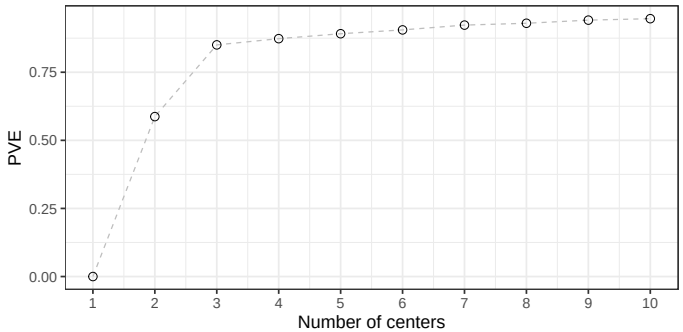
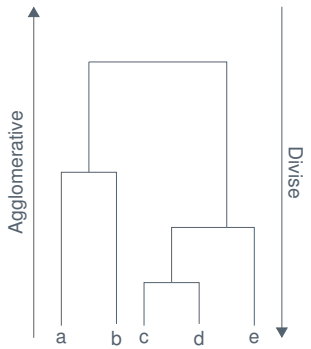


Figure: Scree plot showing the number of clusters against percentage of variance explained.

Clustering
Hierarchical Clustering

Hierarchical clustering is a method which seeks to build a hierarchy of clusters.
In general there are two approaches to obtain this hierarchy, starting from the bottom or from the top (so to speak):

1. **Agglomerative**: This is the bottom up approach, it starts by having each observation in its own cluster and then it merges the most similar together.
2. **Divise**: This is the top down approach, it start by putting all observations in one cluster and then splits recursively to obtain more and more homogenous clusters.



Clustering
Linkages

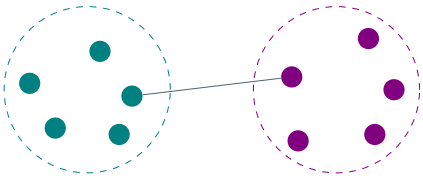
In order to quantify the similarity between observations we need to establish a dissimilarity measure. However there are many ways to define dissimilarity, or linkage, between groups of observations.

1. **Single**: The smallest pairwise dissimilarity.
2. **Complete**: The largest pairwise dissimilarity.
3. **Average**: The average dissimilarity between observations.
4. **Centroid**: The dissimilarity between centroids of clusters.[1]

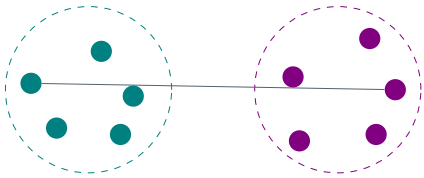
Another consideration is what distance measure to use, typically the Euclidean distance is used, but for other use cases one might opt for the Manhattan distance etc.

[1] Squared distance can cause inversions as we “create” new data points.

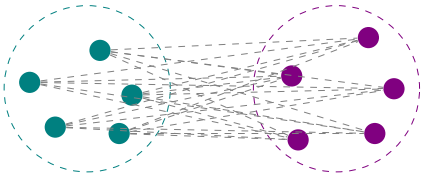
Clustering
Linkages



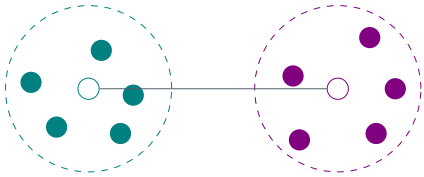
(a) Single.



(b) Complete.



(c) Average.



(d) Centroid.

Figure: The 4 different types of linkages presented on the slide before.

Shrinkage
Variable Selection and Regularization

Because it is often cheaper to obtain multiple observations from a few samples than to obtain more samples, thus increasing the number of explanatory variables in a regression model, a linear regression model would be prone to increasing variance.

When extending linear regression to multiple exaplanatory variables the main objectives is:

- **Model Interpretability**: Models with fewer variables are often more easy to interpret results from and are therefore better to use for decision making.
- **Predition Accuracy**: If by introducing some bias we are able to dramatically improve prediction accuracy, this would be worth considering (bias-variance tradeoff).

Shrinkage
Variable Selection and Regularization

There are multiple tools we can use in this pursuit

- **Subset Selection**: Works by fitting lots of models with different combinations of predictors. Then we can find out which variables are most related to the response and we can select these.
- **Dimensionality Reduction**: Works by projecting explanatory variables into a smaller dimensional space and use these projections as predictors.
- **Shrinkage Methods**: Works by fitting a model using all predictors while shrinking coefficients towards zero, to reduce variance. Some shrinkage methods can also perform variable selection by shrinking coefficients to exactly zero.

Shrinkage
Variable Selection and Regularization

This presentation will focus on shrinkage methods. The two main shrinkage methods are

- **Ridge Regression**
- **Lasso**

They both penalize the “size” of the estimated parameters, however they difer in the way they quantify the “size”. Ridge regression penalize the ℓ_2 norm while Lasso penalize the ℓ_1 norm.

Therefore we can also refer to the two methods as ℓ_1- and ℓ_2-regularizations.

Shrinkage
Ridge Regression

The expression that ridge regression looks to minimize is the following

$$\underbrace{\sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right)^2}_{RSS} + \underbrace{\lambda\sum_{j=1}^{p}\beta_j^2}_{Penalty}, \tag{5}$$

where λ is a parameter that needs to be determined seperately, this is usually done by cross validation.

When $\lambda = 0$ there is no penalty and we are just doing linear regression (OLS). If $\lambda \to \infty$ then β_0 will approach the mean and $\beta_j \to 0$.

Shrinkage

Variable Selection and Regularization

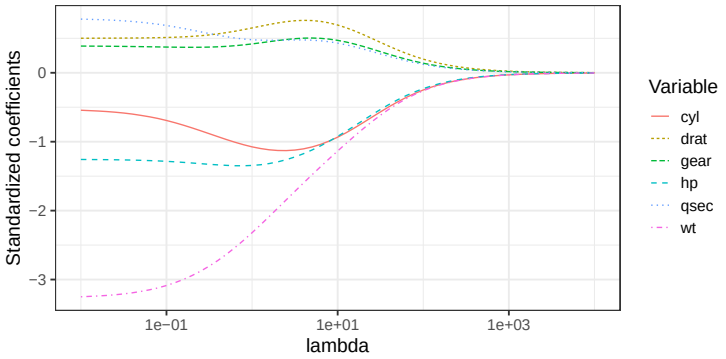


Figure: The effect of λ on coefficents in a ridge regression model for the `mtcars` dataset.

Shrinkage
Variable Selection and Regularization

A benefit of ridge regression is that it can be solved analytically, as the minimization problem is

$$RSS(\lambda) = (\mathbb{Y} - \mathbb{X}\beta)^\top(\mathbb{Y} - \mathbb{X}\beta) - \lambda\beta^\top\beta. \tag{6}$$

If we the above function be the lagrange function, differentiate w.r.t. β and set this equal to zero we find that

$$\hat{\beta}^R = (\mathbb{X}^\top\mathbb{X} + \lambda I)^{-1}\mathbb{X}^\top\mathbb{Y}. \tag{7}$$

It is easy to compute as it is just a closed form expression and we can again observe that for $\lambda = 0$ we get the OLS estimate.

Shrinkage
Lasso

The expression that lasso looks to minimize is the following

$$\sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right)^2 + \lambda\sum_{j=1}^{p}|\beta_j|,$$

where λ, again, is a parameter that needs to be determined seperately.

As opposed to ridge regression, lasso can force coefficients to exactly zero and thereby perform variable selection.

Shrinkage
Lasso

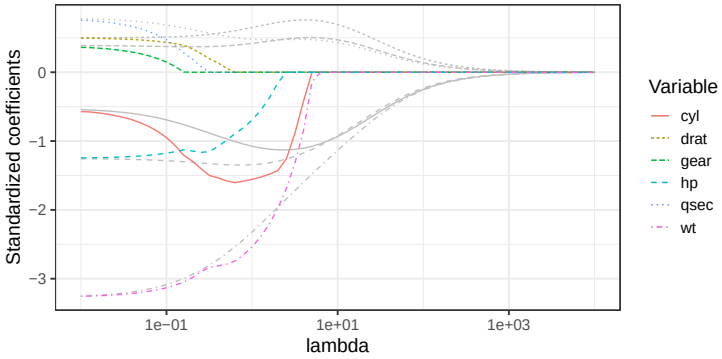


Figure: The effect of λ on coefficents in a lasso regression model for the `mtcars` dataset. Ridge coefficients are included as gray lines for reference.

Shrinkage
Lasso

Unlike ridge regression, there does not exists an analytical solution for the lasso estimates. This is because the absolute value is **not** differentiable.

Therefore we must resort to numerical optimization.

For this we can use a method called **coordinate descent**, that works in the following way:

Instead of trying to solve for all parameters at once we will look for a solution one dimension at a time. When we are done with one dimension we go to the next and then iterate through until we converge.

Shrinkage
Lasso

For the following computations we will assume that the data have been demeaned so we can disregard β_0.

We then start the coordinate descent by the following minimization problem (orange term is just to simplify computation, N is the number of observations and p is the number of variables)

$$\min_{\beta_j} \left\{ \frac{1}{2N} \sum_{i=1}^{N} \left(y_i - \sum_{j=1}^{p} x_j \beta_j \right)^2 + \lambda \sum_{j=1}^{p} |\beta_j| \right\}. \tag{8}$$

Let us define a function L as

$$L = \frac{1}{2N} \sum_{i=1}^{N} \left(y_i - \sum_{j=1}^{p} x_j \beta_j \right)^2 + \lambda \sum_{j=1}^{p} |\beta_j| \tag{9}$$

Shrinkage
Lasso

If we then differentiate w.r.t. β_k we get

$$\frac{\partial L}{\partial \beta_k} = N^{-1} \sum_{i=1}^{N} \left(y_i - \sum_{j=1}^{p} x_j \beta_j \right) (-x_k) + \lambda \underbrace{\partial |\beta_k|}_{\text{Subgradient}} \tag{10}$$

$$= N^{-1} \sum_{i=1}^{N} \left(y_i - \sum_{j \neq k}^{p} x_j \beta_j - x_k \beta_k \right) (-x_k) + \lambda \partial |\beta_k| \tag{11}$$

$$= N^{-1} \sum_{i=1}^{N} \left(y_i - \sum_{j \neq k}^{p} x_j \beta_j \right) (-x_k) + N^{-1} \beta_k \sum_{i=1}^{N} x_k^2 + \lambda \partial |\beta_k| \tag{12}$$

We can define the purple term as $r_k = y_i - \sum_{j \neq k}^{p} x_j \beta_j$ as this is the residual from the model w.o. the k'th regressor.

Shrinkage
Lasso

We can then write

$$= -N^{-1} \sum_{i=1}^{N} (r_k x_k) + N^{-1} \beta_k \sum_{i=1}^{N} x_k^2 + \lambda \partial |\beta_k| \tag{13}$$

$$= -N^{-1} r_k^\top x_k + N^{-1} x_k^\top x_k \beta_k + \lambda \partial |\beta_k|, \tag{14}$$

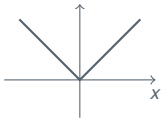
So now we need to figure out what to do with the subgradient.

Shrinkage
Lasso

As there are lots of lines tangent to the absolute value in zero, we can summarize the subgradient as

$$\lambda \partial |\beta_k| = \begin{cases} -\lambda & \text{if } \beta_k < 0 \\ [-\lambda, \lambda] & \text{if } \beta_k = 0 \\ \lambda & \text{if } \beta_k > 0 \end{cases}, \tag{15}$$

for $\beta_k = 0$ the gradient can take all values between -1 and 1.



(a) $f(x) = |x|$.

(b) $\partial f(x)$.

Figure: The absolute value and its gradient.

Shrinkage
Lasso

This means that we can rewrite the derivative as the following

$$\frac{\partial L}{\partial \beta_k} = \begin{cases} -N^{-1} r_k^\top x_k + N^{-1} x_k^\top x_k \beta_k - \lambda & \text{if } \beta_k < 0 \\ [-N^{-1} r_k^\top x_k - \lambda, -N^{-1} r_k^\top x_k + \lambda] & \text{if } \beta_k = 0 \\ -N^{-1} r_k^\top x_k + N^{-1} x_k^\top x_k \beta_k + \lambda & \text{if } \beta_k > 0 \end{cases}. \tag{16}$$

Setting this equal to zero and solving for β_k in the 3 cases gives us the estimates, we take the case $\beta_k < 0$ as an example

$$\frac{\partial L}{\partial \beta_k} = 0 \Leftrightarrow -N^{-1} r_k^\top x_k + N^{-1} x_k^\top x_k \beta_k - \lambda = 0 \tag{17}$$

$$N^{-1} x_k^\top x_k \beta_k = N^{-1} r_k^\top x_k + \lambda \tag{18}$$

$$\beta_k = \left(N^{-1} x_k^\top x_k\right)^{-1} \left(N^{-1} r_k^\top x_k + \lambda\right). \tag{19}$$

Shrinkage
Lasso

Note that

$$\beta_k < 0 \quad \Leftrightarrow \quad N^{-1} r_k^\top x_k + \lambda < 0 \quad \Leftrightarrow \quad N^{-1} r_k^\top x_k < -\lambda. \tag{20}$$

Ultimately we find that, these are the values to update parameters by

$$\hat{\beta}_k = \begin{cases} \left(N^{-1} x_k^\top x_k\right)^{-1} \left(N^{-1} r_k^\top x_k + \lambda\right) & \text{if } N^{-1} r_k^\top x_k < -\lambda \\ 0 & \text{if } -\lambda \leq N^{-1} r_k^\top x_k \leq \lambda \\ \left(N^{-1} x_k^\top x_k\right)^{-1} \left(N^{-1} r_k^\top x_k - \lambda\right) & \text{if } N^{-1} r_k^\top x_k > \lambda \end{cases}, \tag{21}$$

and we remember that r_k is the residual from the model w.o. the k'th regressor.

Shrinkage
Elastic Net

The method is a compromise between Ridge Regression and Lasso as it minimizes

$$\sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right)^2 + \lambda\sum_{j=1}^{p}\left(\alpha|\beta_j| + (1-\alpha)\beta_j^2\right),$$

note that here we have the additional parameter α that determines the weighting of the two norms.

Shrinkage
Elastic Net

- The figure illustrates the feasible region, in the case of two variables, on the RSS surface.
- Most likely the OLS estimate will be somwhere outside the shapes plotted.
- A lasso estimate is more likely to be at the edges.
- Elastic net keeps the pointy edges but rounds the sides (depending on α).
- Elastic net performs variable selection like the lasso, but shrinks correlated regressors like ridge.

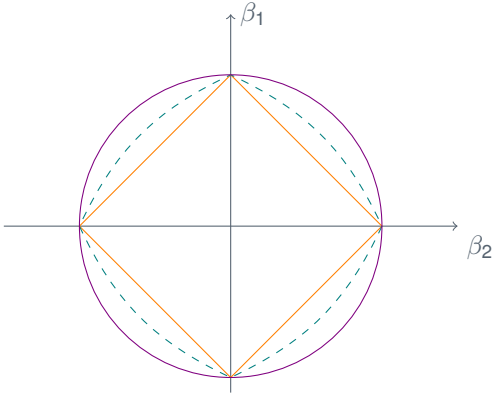


Figure: The feasible region for ridge, lasso and elastic net ($\alpha = .5$).

Shrinkage
Scaling of variables

For both shrinkage methods it is important to scale the variables before fitting the model.

Contrary to linear regression where the scaling of variables are absorbed in the coefficients, this will affect the penalty term for both shrinkage methods.

For example if a variable takes very large values it will get a higher penalty than a variable that takes small values, just because of the unit of measurement.

Classification
Introduction

If the response variable is categorical (qualitative), i.e. it is of the form $y \in \{1, \ldots, L\}$. Then a linear model of the form

$$y = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p,$$

is generally not a good approach to take as it could predict invalid values and for certain types of categorical data there might not be a clear ordering.

Therefore when dealing with categorical variable the aim of the model is to predict the probability that an observation belongs to a certain category, rather than the category itself.

Classification
Logistic Regression

To begin with let us assume the simple case that $y \in \{0, 1\}$ and that we would like to model

$$p(Y = 1|X_i) = p(X_i) = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p = X_i \mathbb{B}. \tag{22}$$

Given that we know probabilities lie between 0 and 1, we would like to transform the linear function such that the output is between 0 and 1.

The most popular, although there are several, would be the logistic function

$$p(X_i) = \frac{e^{X_i \mathbb{B}}}{1 + e^{X_i \mathbb{B}}}. \tag{23}$$

For $X_i \beta \to \infty$ then $p(X_i) \to 1$ and for $X_i \beta \to -\infty$ then $p(X_i) \to 0$.

Classification
Linear Discriminant Analysis (LDA)

Suppose we have a dataset with a response variable $y \in \{0, \ldots, L\}$, explanatory variables $x_1, \ldots, x_p$ and that we would like to model

$$P(y = k|X) = \underbrace{\frac{P(y = k)P(X|y = k)}{P(X)}}_{\text{Bayes Theorem}} = \frac{\pi_k f_k(x)}{\sum_{i=1}^{K} f_i(x)}, \tag{24}$$

where $\pi_k = P(y = k)$ and $f_k(x) = P(X|y = k)$.

If we use the proportion of observations in the dataset that belong to class k as an estimate for π_k, then we just need to model $f_k(x) = P(X|y = k)$.

In other words we need to make some assumption on the distribution of $f_k(x)$.

Classification
Linear Discriminant Analysis (LDA)

The assumption made in LDA is that each $f_k(x)$ come from a multivariate normal distribution, i.e.

$$f_k(x) = \frac{1}{(2\pi)^{p/2}|\Sigma_k|^{1/2}} \exp\left\{-\frac{1}{2}(x-\mu_k)^\top \Sigma_k^{-1}(x-\mu_k)\right\}. \tag{25}$$

Another assumption made in LDA is that $\Sigma_k = \Sigma \; \forall k \in \{1, \ldots, K\}$, in other words all classes will have the same variance-covariance matrix.

Classification
Linear Discriminant Analysis (LDA)

When we classify a new observation, X_0, we simply find the category with the highest probability, $P(y = k|X_0)$ for $k = 1, \ldots, K$.

In other words we want to find the k such that $P(y = k|X)$ is maximized. Since the logarithm is an increasing function we know that the k which maximizes $P(y = k|X)$ also maximizes the following

$$\log(P(y = k|X)) = \log(\pi_k) + \log(f_k(x)) - \underbrace{\log\left(\sum_{i=1}^{K} \pi_i f_i(x)\right)}_{\text{Does not depend on } k}, \tag{26}$$

The last term is identical across categories and we drop this term for the maximization problem.

Classification
Linear Discriminant Analysis (LDA)

So now we have the following

$$\log(\pi_k) + \log(f_k(x)), \tag{27}$$

but let us take a look at the second term. By the normality assumption we have that

$$f_k(x) = \frac{1}{(2\pi)^{p/2}|\Sigma|^{1/2}} \exp\left\{-\frac{1}{2}(x-\mu)^\top \Sigma^{-1}(x-\mu_k)\right\}. \tag{28}$$

Thus we can write (27) as

$$\log(\pi_k) + \underbrace{\log((2\pi)^{p/2}|\Sigma|^{1/2})}_{\text{Does not depend on } k} - \frac{1}{2}(x-\mu)^\top \Sigma^{-1}(x-\mu_k), \tag{29}$$

and subsequently drop another term that is identical across categories.

Classification
Linear Discriminant Analysis (LDA)

So now we have the following

$$\log(\pi_k) - \frac{1}{2}(x-\mu)^\top \Sigma^{-1}(x-\mu_k), \tag{30}$$

again taking a look at the second term

$$(x-\mu_k)^\top \Sigma^{-1}(x-\mu_k) = \underbrace{x^\top \Sigma^{-1} x}_{\text{Does not depend on } k} - x^\top \Sigma^{-1}\mu_k - \mu_k^\top \Sigma^{-1} x + \mu_k^\top \Sigma^{-1}\mu_k, \tag{31}$$

and furthermore we have that $x^\top \Sigma^{-1}\mu_k = \mu_k^\top \Sigma^{-1} x$ because both are scalars and one is just the transpose of the other.

Classification
Linear Discriminant Analysis (LDA)

So we end up with the following expression, which is called the **linear discriminant function**

$$\delta_k(x) = \log(\pi_k) + x^\top \Sigma^- 1 \mu_k - \frac{1}{2}\mu_k^\top \Sigma^{-1} \mu_k, \tag{32}$$

this is what we will use to classify observations. Note the expression is linear in x and therefore we call it linear discriminant analysis.

Classification
Linear Discriminant Analysis (LDA)

In practice the parameters are estimated by

$$\hat{\pi}_k = \frac{n_k}{n}, \quad \hat{\mu}_k = \frac{1}{n_k} \sum_{y_i = k} x_i, \quad \hat{\Sigma} \frac{1}{n - K} \sum_{k=1}^{K} \sum_{y_i = k} (x_i - \hat{\mu}_k)(x_i - \hat{\mu}_k)^\top, \tag{33}$$

i.e. the proportion of observations in class k, the mean for class k and the mean of the variances respectively.

Classification
Quadratic Discriminant Analysis (QDA)

Imagine now that we relax the LDA assumption that $\Sigma_k = \Sigma \; \forall k \in \{1, \ldots, K\}$ and allow classes to have their own variance-covariance matrix.

This implies that some of the simplification we performed before no longer holds and the discriminant function will now take the form

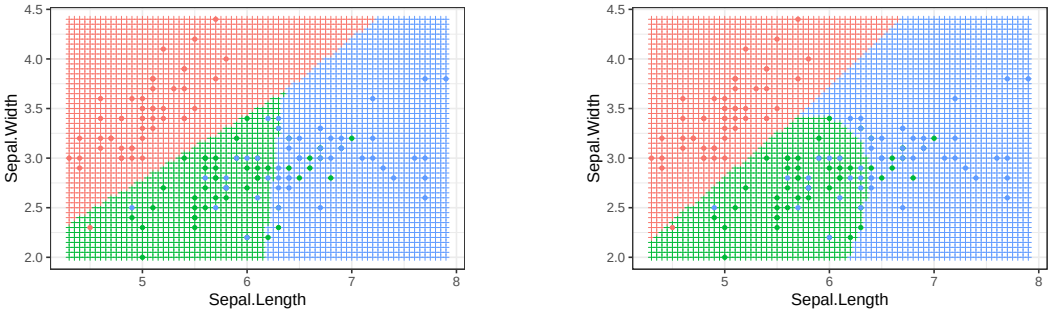
$$\delta_k(x) = -\frac{1}{2} x^\top \Sigma_k x + \log(\pi_k) + x^\top \Sigma_k{}^{-1} \mu_k - \frac{1}{2} \mu_k^\top \Sigma_k{}^{-1} \mu_k - \frac{1}{2} \log |\Sigma_k|, \tag{34}$$

note that first term is quadratic in x.

Another difference in the estimation of the covariance matrices, because we relaxed the assumption we must estimate a variance-covariance matrix for each class

$$\hat{\Sigma}_k = \frac{1}{n_k - 1} \sum_{y_i = k} (x_i - \hat{\mu}_k)(x_i - \hat{\mu}_k)^\top. \tag{35}$$

Classification
Example using the Iris dataset



(a) LDA classification regions.

(b) QDA classification regions.

Figure: Classification regions for LDA and QDA performed on the *Iris* dataset, considering only the variables *sepal width* and *sepal length*. Note that the LDA boundaries are linear while QDA include a non-linear boundary.

Classification
Example using Auto dataset

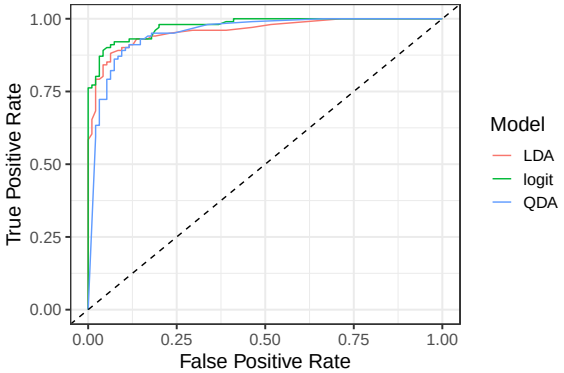


Figure: ROC curves for 3 models on the *auto* dataset from the `ISLR` package. We are predicting whether a car have mpg above the median using displacement, weight, year and horsepower.

Classification
Naive Bayes

The (Naive) Bayes classifier is an example of a parametric classifier (meaning that the number of parameters is fixed), it builds on Bayes theorem

$$P(Y = i|X) = \frac{P(Y = i)P(X|Y = i)}{P(X)}. \tag{36}$$

New data is then assigned to the class with the highest probability given the explanatory variables

$$\hat{Y} = \ arg\ max_i P(Y = i)P(X|Y = i). \tag{37}$$

This means that there are two things we need to model, the first is $P(Y = i)$, but this is simply modelled by the proportions of the dataset.

Classification
Naive Bayes

The second one is $P(X|Y=i)$, note that X is a p-dimensional vector, making the distribution multivariate.

However as estimating multivariate distribution requires lots of computation and suffers from the curse of dimensionality, an assumption in Naive Bayes is that X is independent between classes

$$P(X|Y_i) = P(X_1|Y)P(X_2|Y)\cdots P(X_p|Y). \tag{38}$$

With this assumption we can rewrite

$$P(X|Y=i) = \prod_{j=1}^{p} P(X_j|Y=i), \tag{39}$$

which enables us to estimate all marginal (univariate) distributions one by one.

Classification
Naive Bayes

Typically the we assume that the ditributions are normal, but we can also use others and even seperate distributions for each explanatory variable.

In the case of normally distributed variables we only need to estimate the mean and variance as $X_j|Y = i \sim N(\mu_{j,i}, \sigma^2_{j,i})$, where we use the usual estimates

$$\mu_{j,i} = \frac{1}{N_i} \sum_{x_k|y_k=i} x_{j,i}, \quad \sigma^2_{j,i} = \frac{1}{N_i} \sum_{x_k|y_k=i} (x_{j,i} - \mu_{j,i})^2. \tag{40}$$

Despite the assumption of independence the method tends to work well in practice, although if the assumption is clearly not true we will get biased estimator.

Trees
Introduction

Tree-based methods are supervised learning methods which can be used for both regression and classification.

They work by segmenting the space into a number of simple regions and then, typically, use the mean of the region to make predictions.

Because the segmentation of the space can be summarized in a tree, we call these methods tree-based.

Trees
Classification and Regression Trees (CART)

The purpose of the CART algorithm is to decide on the split points. This is done in a greedy way one split at a time, as the task of checking all possible combinations of splits would be computationally infeasible.

We look for split points by solving (here we assume that the loss function in the ℓ_2 norm)

$$\min_s \left[\min_{c_1} \sum_{x_i < s} (y_i - c_1)^2 + \min_{c_2} \sum_{x_i \geq s} (y_i - c_2)^2 \right],$$

so we wish to find a split point s that minimizes the loss function on either side. Recall that

$$\tilde{y}_1 = min_{c_1} \sum_{x_i < s} (y_i - c_1)^2 \text{ and } \tilde{y}_2 = min_{c_2} \sum_{x_i \geq s} (y_i - c_2)^2.$$

Where $\tilde{y}_1$, $\tilde{y}_2$ are the means for y_i such that $x_i < s$ and $x_i \geq s$ respectively.

Trees
Classification and Regression Trees (CART)

The split points we find produces basis functions $b_1(x) = I(x_i < s)$ and $b_2(x) = I(x_i \geq s)$, which would be equivalent to fitting the model

$$y_i = \beta_1 b_1(x_i) + \beta_2 b_2(x_i). \tag{41}$$

Next step is to repeat the same procedure in the new regions, that is we find the best split points in each of the new regions and the choose the best.

We do this until hit some predetermined stopping criteria, could be minimum number of observations in each region, not enough increase in fit etc.

Trees

Classification and Regression Trees (CART)

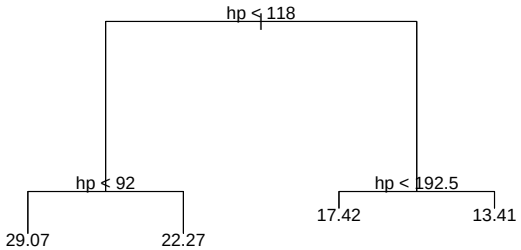


Figure: A decision tree explaining *miles per gallon* by *horsepower*.

Trees
Classification and Regression Trees (CART)

For the univariate case it is pretty straigth forward, but what if we have more variables?

It is still pretty straightforward, so the idea is to obtain possible cuts for each variable and the choose the best. Then we get two regions and we repeat the same procedure in each. This method is called **recursive binary splitting**.

Formally this can be expressed as, first defining regions

$$R_1(j,s) = \{X|X_j < s\}, \quad R_2(j,s) = \{X|X_j \geq s\}, \tag{42}$$

then finding the cutpoint amounts to solving

$$\min_{j,s} \left[\sum_{\{i|x_i \in R_1(j,s)\}} (y_i - \tilde{y}_{R_1})^2 + \sum_{\{i|x_i \in R_2(j,s)\}} (y_i - \tilde{y}_{R_2})^2 \right]. \tag{43}$$

Trees

Classification and Regression Trees (CART)

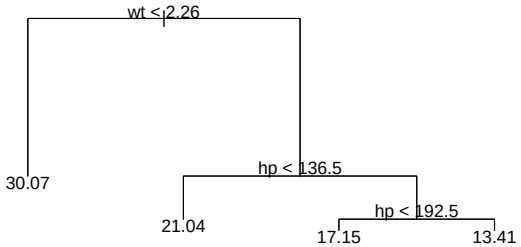


Figure: A decision tree explaining *miles per gallon* by *horsepower* and *weight*.

Trees
Pruning

The next thing we need to consider is whether we are stopping at the **right** time.

1. In general a **larger tree** would fit the data better, but may have **high variance**.
2. Whereas a **smaller tree** may not fit the data well, and thereby have **high bias**.

To deal with the bias-variance tradeoff we do what is called **pruning**. In order to perform the pruning we neeed a large tree, the pruning part is then to find the subtree that leads to the lowest generalization (out-of-sample) error.

One way is to go through all subtrees, but this will not scale to large trees.

To do this in a more time sensible manner we use a greedy approach, this is called **weakest link pruning** and works by always pruning the cheapest split (in terms of the loss).

Trees
Pruning

This is done by minimizing (for $\alpha \geq 0$)

$$C_\alpha(T) = \sum_{m=1}^{|T|} \sum_{\{i|x_i \in R_m\}} (y_i - \hat{y}_{R_m})^2 + \alpha|T|, \tag{44}$$

where $|T|$ denotes the number of leafs and R_m is the region corresponding the m'th leaf.

- The orange term relates to **how well we fit the data**,
- The purple term is a **penalty of the complexity**.

Trees
CART Algorithm

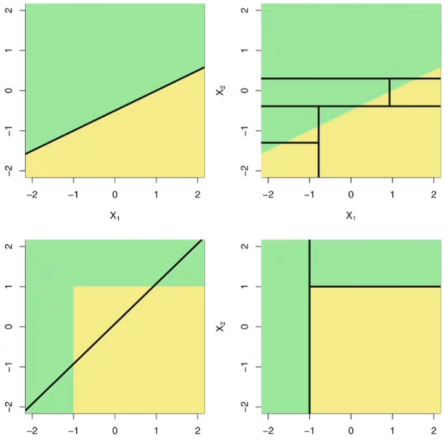
The algorithm of CART can be descriped by the following steps;

1. Use **recursive binary splitting** to grow a large tree on the training data, stopping only when each terminal node has fewer than some minimum number of observations.
2. Apply **weakest link pruning** to the large tree in order to obtain a sequence of best subtrees as a function of α.
3. Use K-fold cross-validation to choose α.
4. Return the **subtree from step 2**, that corresponds to the chosen value of α.

To use CART for classification we need to choose a proper loss function, could be missclassification error, Gini index, cross-entropy etc.

Trees
Comparing Linear Regression and CART

- So how do CART compare to linear regression?
- Well it depends on the data.



Trees
Comparing Linear Regression and CART

Consider the following model (non-binary)

$$y = 1 + 2x_1 + 3x_2 + \varepsilon, \tag{45}$$

where $x_1, x_2 \sim N(0,1)$ and $\varepsilon \sim N(0, 1/2)$. We can then introduce the variables $\tilde{x}_1, \tilde{x}_2$ given by

$$\tilde{x}_1 = \begin{cases} 1 & \text{for } x_1 > 0 \\ 0 & \text{for } x_1 \leq 0 \end{cases}, \quad \tilde{x}_2 = \begin{cases} 1 & \text{for } x_2 > 0 \\ 0 & \text{for } x_2 \leq 0 \end{cases}, \tag{46}$$

and proprose a separate model (binary)

$$\tilde{y} = 1 + 2\tilde{x}_1 + 3\tilde{x}_2 + \varepsilon. \tag{47}$$

We can then compare how the CART algorithm compares to linear regression on both the binary and non-binary model.

Trees
Comparing Linear Regression and CART

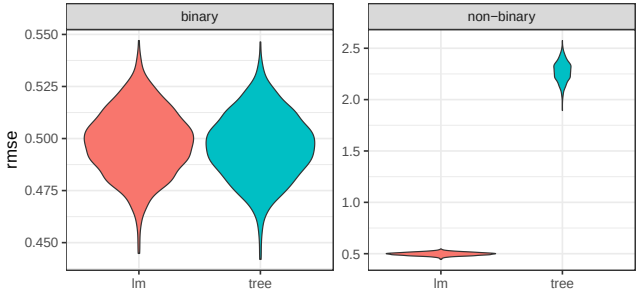


Figure: Comparing linear regression (`lm` from `base R`) and CART (`tree` from the `tree` package) on 1000 repetions of 500 observations. We see that when the data is generated from a step function its a tie between `tree` and `lm`, but when the data is linear the CART understandably struggles compared to linear regression.

Trees
Summary of CART

In general the procedure is simple and easy to interpret, handles categorical variables, perform variable selection.

Unfortunately it is also unstable, meaning a few observations can dramatically impact the outcome of the model.

There exists several methods to overcome these disadvantages

1. **Bagging**
2. **Random Forest**
3. **Boosting**

Trees
Bagging

Bagging (Bootstrap Aggregation) is a method used to **reduce the variance** of an algorithm.

This is done by taking a number of random samples with replacement (**bootstrap samples**) from the dataset and the fitting a tree on each of the samples.

Formally we calculate B trees, $\hat{f}^1(x), \hat{f}^2(x), \ldots, \hat{f}^B(x)$, using separate bootstrap samples. Then to get the final prediction we take either the average or a majority vote

$$\hat{f}_{avg}(x) = \frac{1}{B}\sum_{j=1}^{B}\hat{f}^j(x), \quad \hat{f}_{avg}(x) = \ arg\ max_k \sum_{j=1}^{B}\mathbf{1}(\hat{f}^j(x) = k). \tag{48}$$

The parameter B is not critical as increasing it will not lead to overfitting.

Trees
Bagging

Bagging gets improved accuracy when compared to a single tree, but we lose the interpretability we have with a single tree and we need to resort to measures of variable importance when trying to determine the important variables.

Variance is reduce because of the averaging, but as much of the data is shared between samples the predictions will be highly dependent. So one could imagine reducing the variance even more if we could obtain less dependent predictions.

This is the idea behind the next method **Random Forest**.

Trees
Random Forest

In the case of a **single strong predictor in the dataset**, most or all of the trees obtained from bagging would split on this variable first and most **trees would be quite similar**.

The basic principle is the same as in bagging, the difference is that when constructing a new tree we take a **random sample of the predictors**, of size m, to use in the construction.

Note that if we have p predictors and $m = p$ we get bagging, so we could interpret bagging as random forest but selecting all predictors each time.

Trees
Boosting

- The last method is fundamentally different from the other two.
- There are no chance, instead we try to iteratively improve the fit.
- Number of trees B is related to the shrinkage λ.
- The parameter d controls the complexity of the trees in the ensemble, often a small number, like $d = 1$ is sufficient.
- Risk of overfitting with too large B or too low λ, can be controlled with cross validation.

1. Set $\hat{f}(x) = 0$ and $r_i = y_i$ for all i in the training set.
2. For $b = 1, 2, \ldots, B$ repeat
   - 2.1 Fit a tree $\hat{f}^b$ with d splits to the training data (X, r)
   - 2.2 Update $\hat{f}$ by adding in a shrunken version of the new tree:
   $$\hat{f}(x) \leftarrow \hat{f}(x) + \lambda \hat{f}^b(x).$$
   - 2.3 Update the residuals,
   $$r_i \leftarrow r_i - \lambda \hat{f}^b(x_i).$$
3. Output the boosted model
$$\hat{f}(x) = \sum_{b=1}^{B} \lambda \hat{f}^b(x)$$

Support Vector Machines
Optimal Seperating Hyperplanes

The idea behind optimal seperating hyperplanes is to find a hyperplane, in the span of the explanatory variables, such that observations from different categories lie on different sides of the hyperplane.

If we let $X_1, \ldots, X_p$ be explanatory variables for a binary response variable and define scalars $\beta_0, \beta_1, \ldots, \beta_p$. When then define a hyperplane by points that satisfy

$$\beta_0 + \beta_1 X_1 + \cdots \beta_p X_p = 0. \tag{49}$$

As the coding for the two classes in arbitrary we can let the response variable $y \in \{-1, 1\}$.

Support Vector Machines
Optimal Seperating Hyperplanes

Then we look for $\beta_0, \beta_1, \ldots, \beta_p$ such that all observations with $y_i = -1$ are on one side and vice versa. More formally this means that we seek coefficients s.t.

$$\beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip} > 0 \text{ if } y_1 = 1, \tag{50}$$
$$\beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip} < 0 \text{ if } y_1 = -1. \tag{51}$$

Giving the encoding we use this can be simplified to

$$y_i \left(\beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip}\right) > 0. \tag{52}$$

Note that if we find such a hyperplane, it would entail that there exists an infinite amount of them. But then how do we find the **best**.

Support Vector Machines

Optimal Seperating Hyperplanes

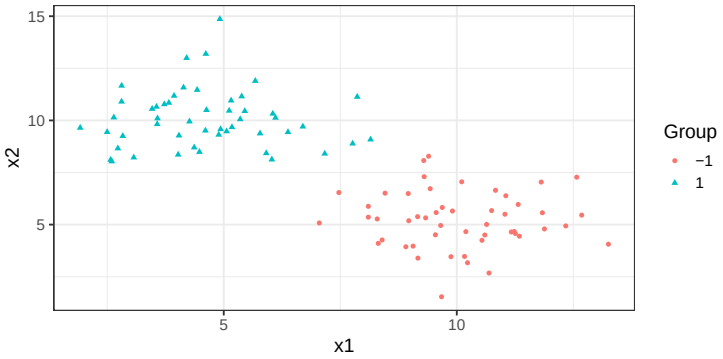


Figure: Data that can be seperated by a hyperplane, but it is not clear which one to use.

Support Vector Machines
Optimal Seperating Hyperplanes

Before we can find the **best** hyperplane, we need to decide what we mean by that. A common criteria is the hyperplane that is **farthest away from the observations**.

Finding the hyperplane that is farthest away from all observations amounts to finding the hyperplane that is farthest from the observation that closest to it. This smallest distance from an observation to the hyperplane is called the **margin**. In other words we look for the hyperplane with **maximal margin**.

Finding the distance to the hyperplane is equivalent to solving, where x_0 is an observation

$$\min_x \|x - x_0\| \text{ subject to } \beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip} = 0. \tag{53}$$

It can be shown that the solution is the orange term and M is the margin

$$M = M(\beta_0, \beta_1, \ldots, \beta_p) = \min_{\{(x_{1i}, \ldots, x_{pi})_{i=1}^n\}} \frac{\beta_0 + \beta_1 x_{1i} + \cdots + \beta_p x_{pi}}{(\beta_1^2 + \cdots + \beta_p^2)^{1/2}}. \tag{54}$$

Support Vector Machines
Optimal Seperating Hyperplanes

Finding then the **maximal hyperplane** can formally be written as

$$\max_{\beta_0,\beta_1,\ldots,\beta_p} M \tag{55}$$

s.t.

$$\underbrace{\sum_{j=1}^{p} \beta_j^2 = 1}_{\text{identification}}, \quad \underbrace{y_i(\beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip}) \geq M \quad \forall i}_{\text{ensure observations are on the correct side}} \tag{56}$$

Note that the hyperplane **only** depends on the observations that are close to it, namely the observations whose distance to the hyperplane is equal to the margin. These observations are called **support vectors**.

Support Vector Machines

Optimal Seperating Hyperplanes

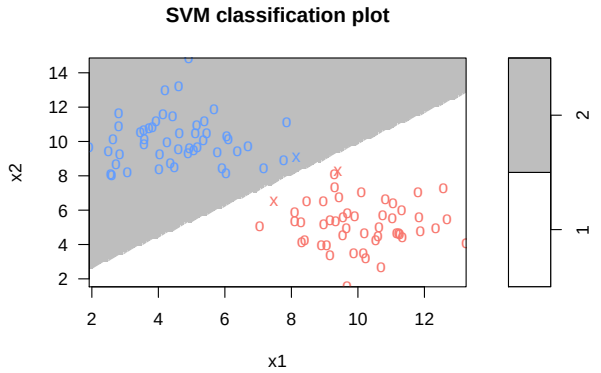


Figure: Maximal hyperplane with support vectors marked with x and obervations with o.

Support Vector Machines
Optimal Seperating Hyperplanes

A big assumption in this framework is that a seperating hyperplane exists, but in many cases it is not possible to perfectly seperate groups and therefore the method cannot be used in these scenarios.

This leads us to the next topic **support vector classifiers**.

Support Vector Machines
Support Vector Classifier

Insted of using a **hard margin**, as with optimal seperating hyperplanes, support vector classifiers uses a **soft margin**. This means that we allow for **some misclassifications**.

Formally what we want to do is

$$\max_{\beta_0,\beta_1,\ldots,\beta_p,\varepsilon_1,\ldots,\varepsilon_n} M \tag{57}$$

s.t.

$$\sum_{j=1}^{p} \beta_j^2 = 1, \quad y_i(\beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip}) \geq M(1 - \varepsilon_i) \quad \forall i, \tag{58}$$

$$\varepsilon_i \geq 0 \quad \forall i, \quad \sum_{j=1}^{n} \varepsilon_j \leq C, \tag{59}$$

where C is a tuning parameter.

Support Vector Machines
Support Vector Classifier

If $\varepsilon_i = 0$, we get the condition from the maximal margin classifier at most on the margin and in the correct group.

If $1 > \varepsilon_i > 0$ the observation is inside of the margin as the distance to the hyperplane is strictly less than M.

If $\varepsilon_i > 1$ the observation is in the wrong group. The restriction changes sign.

The support vectors are observations with $\varepsilon_i > 0$.

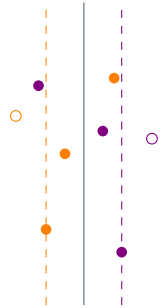


Figure: Illustration of the different possible scenarios of ε_i.

Support Vector Machines

Support Vector Classifier

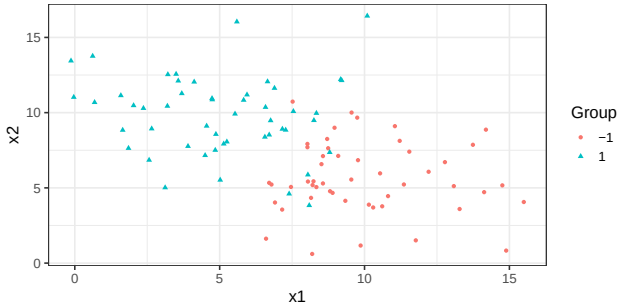


Figure: Overlapping that cannot be perfectly seperated by a hyperplane.

Support Vector Machines
Support Vector Classifier

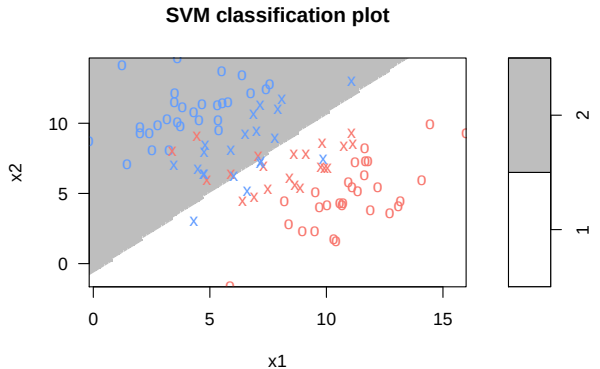


Figure: The result from a support vector classifier, many more support vectors (wider margin).

Support Vector Machines
Support Vector Machines

Support vector machines extends the support vector classifier by allowing **non linear** specifications.

In other words we can add transformations of the data to extend the space in which we are searching for the hyperplane. An example could be adding **polynomial terms**.

The model is still **linear in the transformed variables**, but we are looking for hyperplanes in a higher dimension.

Instead of figuring out what transformation of variables should be used case by case, SVM's use the trick that relates to the optimization problem that is solved.

Without getting to much into it i can say that SVC's use cross-products as a similarity measure between observations (linear kernel). SVM's extend to other **kernels**.

Support Vector Machines

Support Vector Machines

A kernel is a function that quantifies the similarity between observations. There are many possible kernels to use such as

- **Polynomal kernel** - $K(x_i, x_j) = \left(1 + \sum_{k=1}^{p} x_{ik} x_{jk}\right)^d$
- **Radial kernel** - $K(x_i, x_j) = \exp\left(-\gamma \sum_{k=1}^{p} (x_{ik} - x_{jk})^2\right)$
- **Sigmoid kernel** - $K(x_i, x_j) = tanh\left(\kappa \sum_{k=1}^{n} (x_{ik} x_{jk}) + c\right)$

The different kernel all have their own parameter(s) that need to be tuned in order to get the best performance.

Support Vector Machines
Support Vector Machines

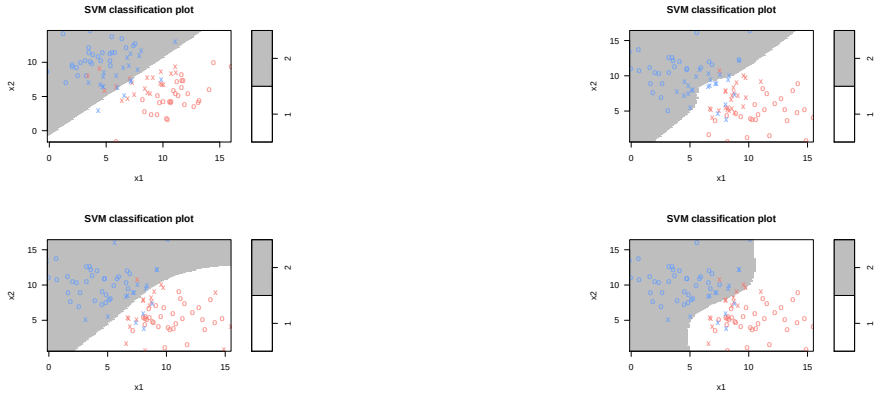


Figure: From the top right; linear, polynomial, radial, sigmoid.

Support Vector Machines
Support Vector Machines

Even though segmentation look non-linear, we note that it is linear in a higher dimensional space we are just not able to see on the plot.

Lastly we can note that the more support vectors there are the more bias, but less variance there are. Remember that this was directly related to C parameter, that dictates how wide the margin is.

So **small** C will give low bias (allow only a few misclassifications) but high variance, where as **large** C will give high bias (allow more misclassifications) but lower variance.

By choosing the loss function appropiately SVM's can also be used for regression.

Neural Networks
Perceptron

The most basic form of a neural network is the **perceptron**.

There are an **input node for each explanatory variable**, the bias term (intercept) and then there are a **single output node**.

A weight is assigned to each of the input nodes and then the **linear combination** of weights times input is fed to the **activation function** in the output layer. For regression we can just use the linear combination.

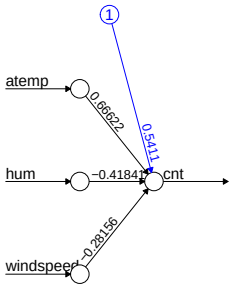


Figure: Perceptron made from the bike sharing dataset.

Neural Networks
Perceptron

The weights are determined, or learned, using a loss function and an iterative approach

$$w_i^{\text{new}} = w_i^{\text{old}} - \eta \frac{\partial L}{\partial w_i}, \tag{60}$$

where the loss function is given by

$$L = \frac{1}{2}(y - \hat{y})^2 = \frac{1}{2}\left(y - g\left(\sum_i w_i x_i\right)\right)^2, \tag{61}$$

$$\frac{\partial L}{\partial w_i} = \left(y - g\left(\sum_i w_i x_i\right)\right)\left(-g'\left(\sum_i w_i x_i\right)\right)(x_i), \tag{62}$$

where we used the chain rule twice. The **learning rate** is denoted by η and a cycle through the weights is called an **epoch**.

Neural Networks
Multilayer Neural Network

The perceptron is a simple linear model, to create a more complex model we introduce **hidden layers**. Each node in the hidden layer is activated by the previous layer

$$a_i^{(1)} = g\left(w_{0i}^{(1)} + \sum_{j=1}^{k^{(0)}} w_{ji}^{(1)} x_j\right), \quad i = 1, \ldots, k^{(1)}. \quad (63)$$

$k^{(i)}$ is the number of nodes in layer i. The output layer is

$$\hat{y} = a_0^{(2)} = g\left(w_0^{(2)} + \sum_{j=1}^{k^{(1)}} w_{j1}^{(2)} a_j^{(1)}\right). \quad (64)$$

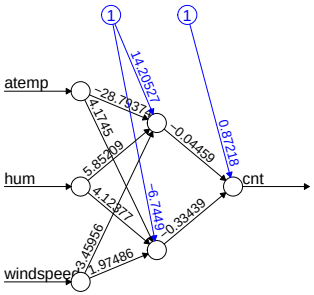


Figure: Multilayer neural network made from the bike sharing dataset.

Neural Networks
Multilayer Neural Network

In more general terms, let us say we have m hidden layers

$$a_i^{(s)} = g\left(w_{0i}^{(s)} + \sum_{j=1}^{k^{(s-1)}} w_{ji}^{(s)} a_j^{(s-1)}\right) \quad \text{for } i = 1, \ldots, k^{(s)}, \tag{65}$$

$$\hat{y} = a_0^{m+1} = g\left(w_0^{(m+1)} + \sum_{j=1}^{k^{(m)}} w_{jm}^{(m+1)} a_j^{(m)}\right). \tag{66}$$

Neural Networks
Estimation of a Multilayer Neural Network

The next thing to consider will be how to **estimate** a multilayer neural network.

Let us say that we have a neural network with m hidden layers and input $(x_i, y_i)_{i=1}^n$, for simplicity we will assume that all bias terms (intercepts) are equal to 1. We want to evaluate the loss function

$$L = \frac{1}{2n} \sum_{i=1}^{n} (\hat{y}_i - y_i)^2, \tag{67}$$

then obtain derivatives $\frac{\partial L}{\partial w_{ij}^{(k)}}$ and update the weights by

$$\Delta w_{ij}^k = -\eta \frac{\partial L}{\partial w_{ij}^{(k)}}. \tag{68}$$

Neural Networks
Backpropagation

In practice this is done by a method called **backpropagation**.

It can be shown that the problem of finding $\frac{\partial L}{\partial w_{ij}^{(k)}}$ can be done for each observation $\frac{\partial L_s}{\partial w_{ij}^{(k)}}$.

Remember the expression for each node $a_i^{(s)} = g\Big(\underbrace{\sum_{j=1}^{k^{(s-1)}} w_{ji}^{(s)} a_j^{(s-1)}}_{z_j^{(s)}}\Big)$, then we have

$$\frac{\partial L_s}{\partial w_{ij}^{(k)}} = \underbrace{\frac{\partial L_s}{\partial z_j^{(k)}}}_{\delta_j^{(k)}} \frac{\partial z_j^{(k)}}{\partial w_{ij}^{(k)}} \quad \textit{by the chain rule} \tag{69}$$

Neural Networks
Backpropagation

The first term, $\delta_j^{(k)}$, depends on the loss and therefore we call it the error term.

For the second term we see that

$$\frac{\partial z_j^{(k)}}{\partial w_{ij}^{(k)}} = \frac{\partial}{\partial w_{ij}^{(k)}} \sum_{t=0}^{k^{(s)}} w_{tj}^{(k)} a_t^{(k-1)} = a_i^{(k-1)}. \tag{70}$$

Thus we ultimately get

$$\frac{\partial L_s}{\partial w_{ij}^{(k)}} = \frac{\partial L_s}{\partial z_j^{(k)}} \frac{\partial z_j^{(k)}}{\partial w_{ij}^{(k)}} = \delta_j^{(k)} a_i^{(k-1)}, \tag{71}$$

We first calculate $a_i^{(k-1)}$ in a forward phase and then $\delta_j^{(k)}$ is a backwards phase.

Neural Networks
Backpropagation

Forward phase:

- The inputs for a training instance are fed into the neural network.
- This results in a forward cascade of computations across the layers, using the current set of weights.
- The final predicted output can be compared to the true value.

Backward phase:

- Use the error estimate to learn the weights in the backward direction, starting with the output node.
- The error estimate of a node in the hidden layer is computed as a function of the error estimates and weights of the nodes in the layer ahead of it.

Neural Networks
Backpropagation

The first step in the backward phase is to compute $\delta_1^{(m+1)}$ (*the output layer*)

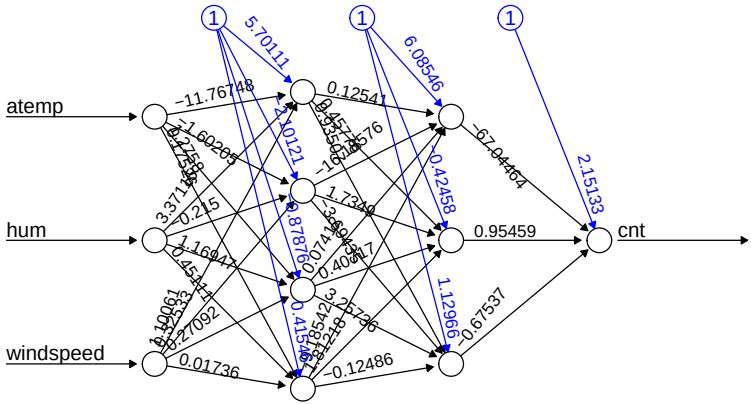
$$\delta_1^{(m+1)} = \frac{\partial L}{\partial z_1^{(m+1)}} = \frac{\partial}{\partial z_1^{(m+1)}} \left(\frac{1}{2} (g(z_1^{(m+1)}) - y)^2 \right) = \left(g(z_1^{(m+1)}) - y \right) g'(z_1^{(m+1)}), \quad (72)$$

The same as for the perceptron. For the hidden layers the error term **depends on subsequent layers**, the chain gives that

$$\delta_j^{(k)} = \frac{\partial L}{\partial z_j^{(k)}} = \sum_i \underbrace{\frac{\partial L}{\partial z_i^{(k+1)}}}_{\delta_j^{(k+1)}} \frac{\partial z_i^{(k+1)}}{\partial z_j^{(k)}} = \sum_i \delta_j^{(k+1)} \frac{\partial z_i^{(k+1)}}{\partial z_j^{(k)}}. \quad (73)$$

We then perform first the forward phase and the backward for each epoch and update the weights (like for the perceptron).

Neural Networks
Backpropagation



Error: 5.868632 Steps: 72377

Neural Networks

Comparing Linear Regression and Neural Networks - Residuals

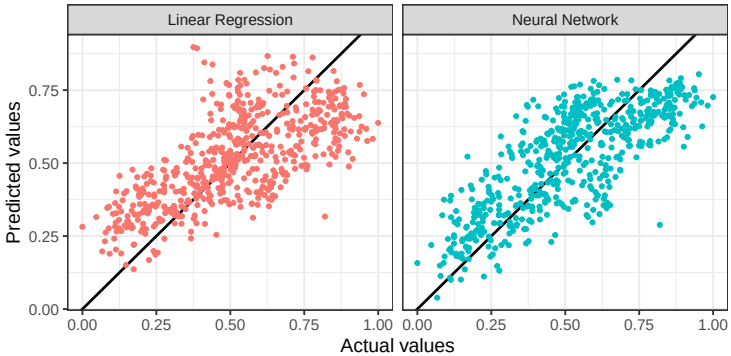


Figure: Comparing linear regression (train RMSE=.141) and a neural network (test RMSE=.163) on the bike sharing dataset.

Neural Networks

Comparing Linear Regression and Neural Networks - Generalization

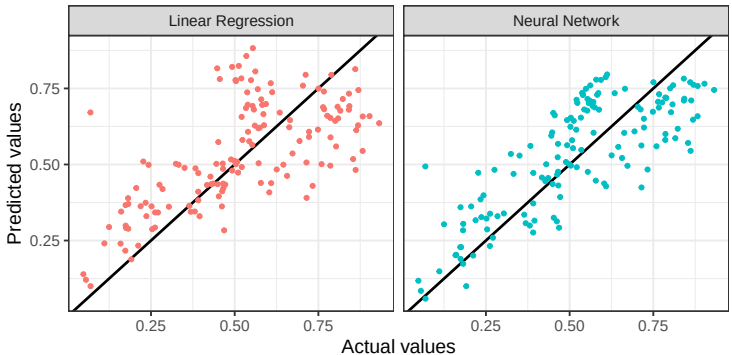


Figure: Comparing linear regression (test RMSE=.133) and a neural network (test RMSE=.166) on the bike sharing dataset.

Neural Networks
Considerations

One must choose learning rate and epochs with caution as the dictate whether we are over- or underfitting the data.

Likewise with the topology of the network, more nodes and layers means that we are better able to fit the data, but we risk overfitting when maybe the network too large.

Size of the network will also have a big impact on the time it takes to train the model, generally we say that neural networks are relatively slow to train compared to other methods.